

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
 Data File : BG051058.D
 Acq On : 16 Nov 2021 2:13
 Operator : CG/JU
 Sample : M4657-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VWE-B31-111121-10-15

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051058.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.762	380	387	399	rBV	778671	1315734	57.09%	9.030%
2	7.378	653	662	675	rBV	805029	1455205	63.15%	9.987%
3	8.224	799	806	818	rVB	167501	301731	13.09%	2.071%
4	9.399	996	1006	1019	rBV	485703	924814	40.13%	6.347%
5	10.556	1197	1203	1215	rVB3	26581	49985	2.17%	0.343%
6	10.797	1236	1244	1254	rBV	62438	121247	5.26%	0.832%
7	11.056	1280	1288	1296	rBV	236754	443886	19.26%	3.046%
8	11.778	1404	1411	1423	rBV	13915	38417	1.67%	0.264%
9	13.476	1690	1700	1707	rBV	1282618	2023264	87.80%	13.886%
10	14.164	1812	1817	1821	rVB4	20020	27770	1.21%	0.191%
11	14.258	1827	1833	1836	rBV2	23281	31011	1.35%	0.213%
12	14.851	1927	1934	1942	rBV	371049	599663	26.02%	4.116%
13	16.344	2181	2188	2199	rVB	859872	1369073	59.41%	9.396%
14	17.601	2396	2402	2408	rBV	424479	659473	28.62%	4.526%
15	18.453	2542	2547	2556	rBV2	69943	127256	5.52%	0.873%
16	18.964	2630	2634	2640	rBV3	28421	43993	1.91%	0.302%
17	19.305	2688	2692	2696	rBV6	11492	23400	1.02%	0.161%
18	19.375	2699	2704	2710	rVV	41403	78921	3.42%	0.542%
19	20.004	2808	2811	2817	rVB	33688	46959	2.04%	0.322%
20	20.186	2837	2842	2849	rBV	1716685	2304529	100.00%	15.816%
21	20.827	2948	2951	2954	rBV2	49895	56106	2.43%	0.385%
22	21.490	3060	3064	3074	rVB2	102628	193849	8.41%	1.330%
23	21.902	3128	3134	3140	rVB2	321499	553690	24.03%	3.800%
24	23.095	3331	3337	3343	rVB	225805	410643	17.82%	2.818%
25	24.270	3532	3537	3544	rVB	99148	213659	9.27%	1.466%
26	25.315	3709	3715	3725	rVB2	150579	451203	19.58%	3.097%
27	26.473	3905	3912	3926	rVB2	222907	705253	30.60%	4.840%

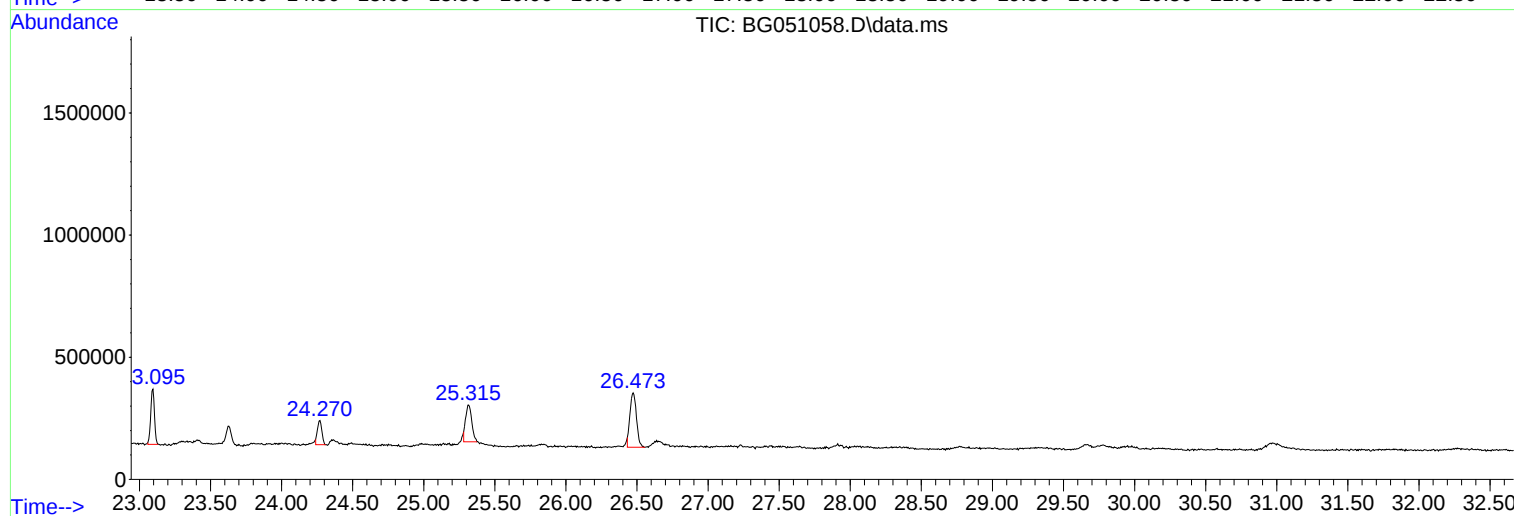
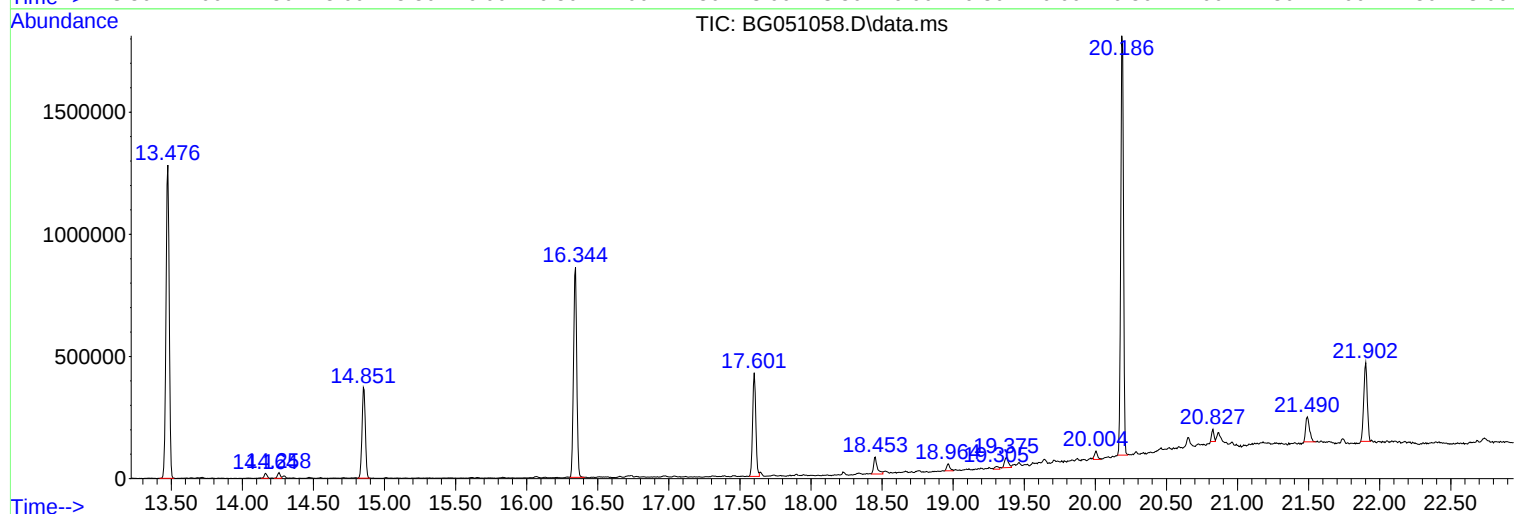
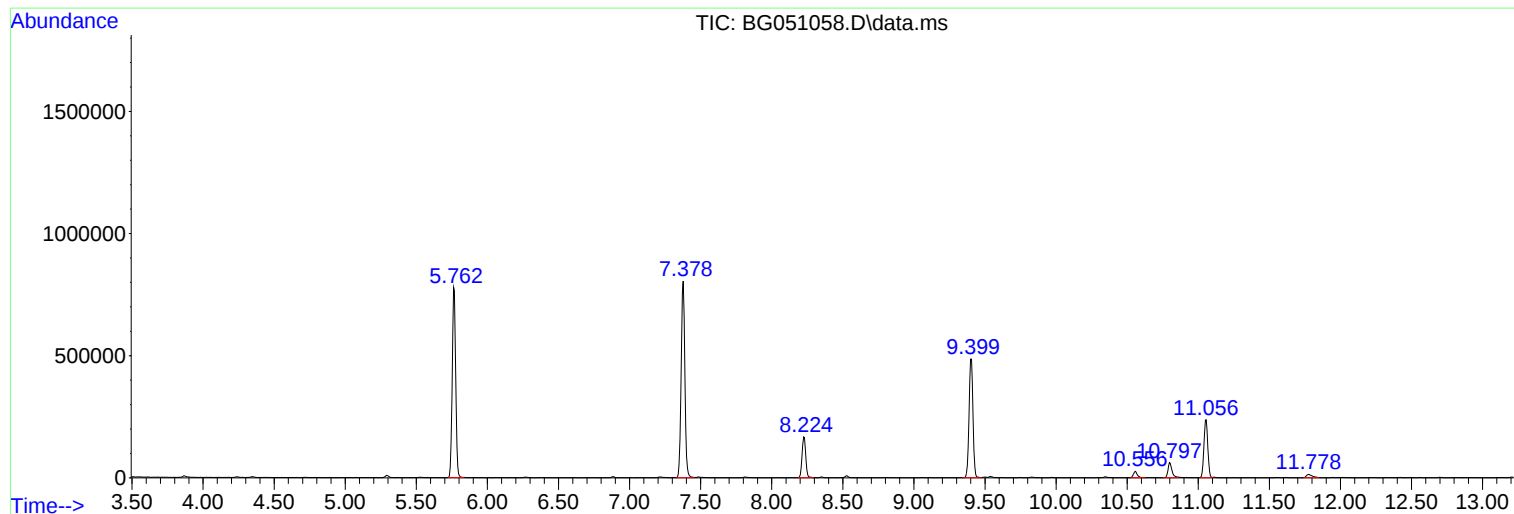
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ClientSampleId :
VWE-B31-111121-10-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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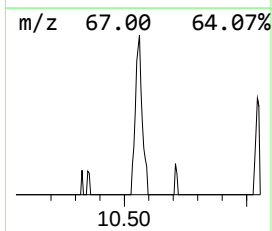
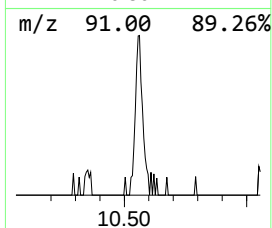
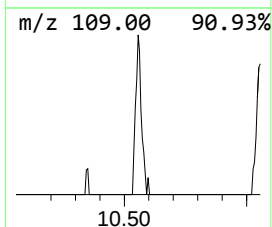
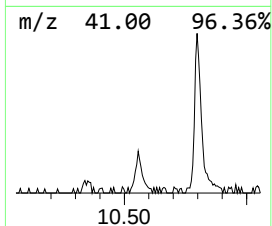
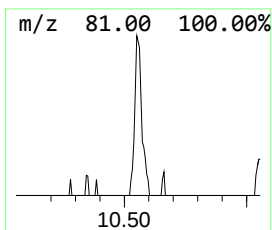
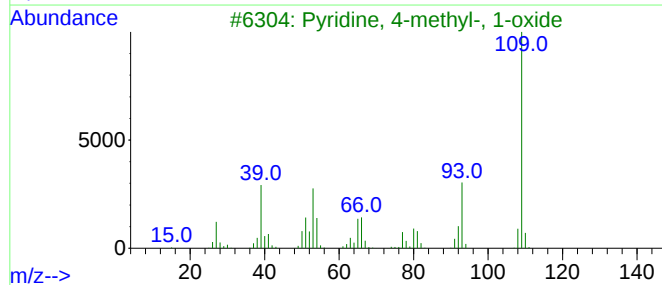
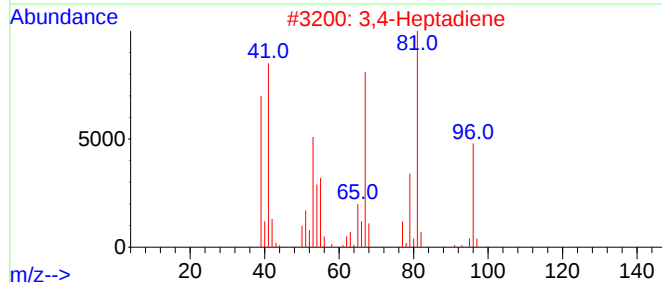
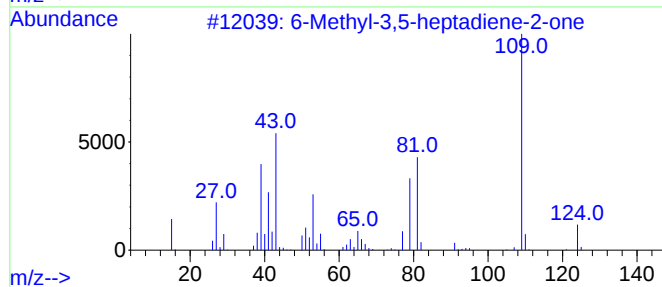
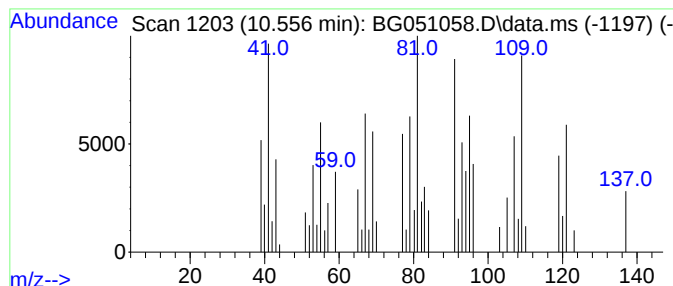
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown10.556 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.556	2.25 ng	49985	Naphthalene-d8	11.056

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		6-Methyl-3,5-heptadiene-2-one	124	C8H12O	001604-28-0	46
2		3,4-Heptadiene	96	C7H12	002454-31-1	45
3		Pyridine, 4-methyl-, 1-oxide	109	C6H7NO	001003-67-4	45
4		2,5-Heptadiene, (E,E)-	96	C7H12	039619-60-8	43
5		1,3-Pentadiene, 2,4-dimethyl-	96	C7H12	001000-86-8	43



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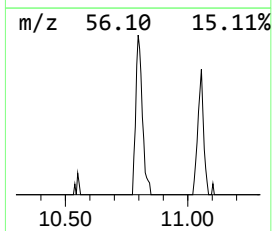
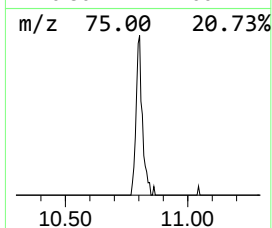
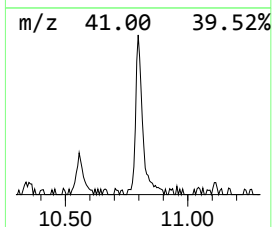
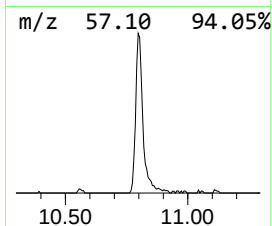
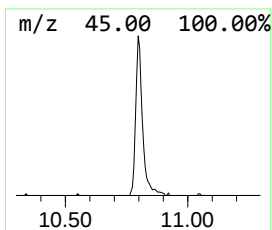
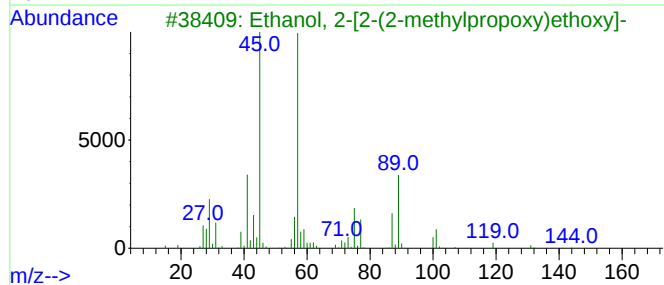
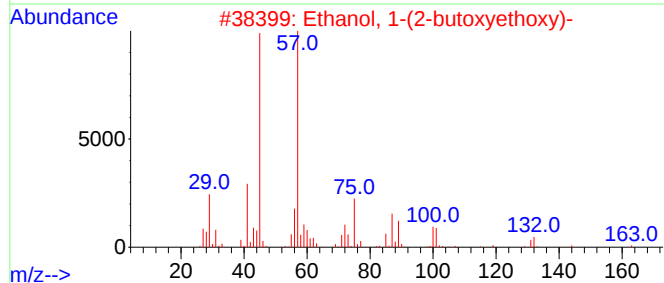
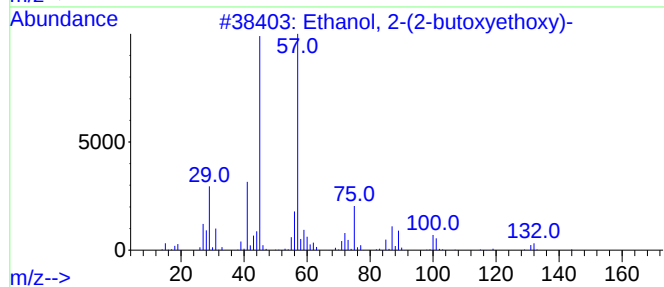
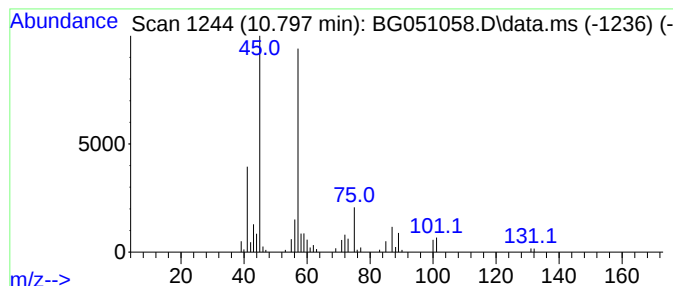
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.797	5.46 ng	121247	Naphthalene-d8	11.056

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			(S)-Methyl 2,3-dihydroxypropanoa...	134	C5H10O4	354578-58-8	50
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	47



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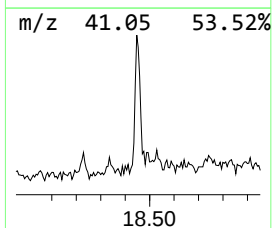
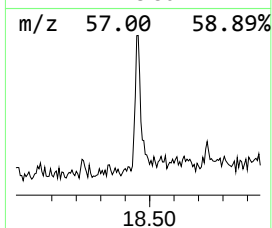
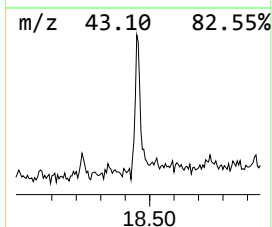
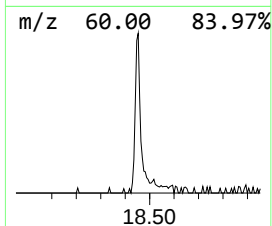
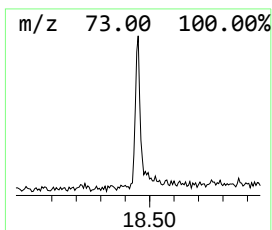
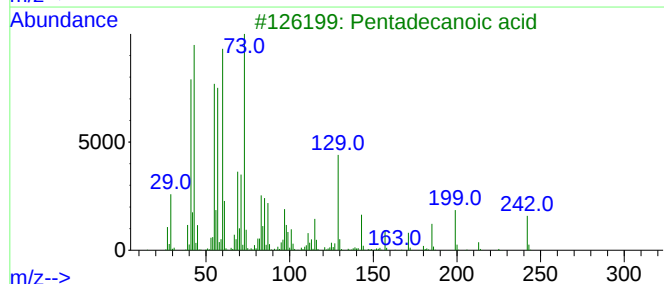
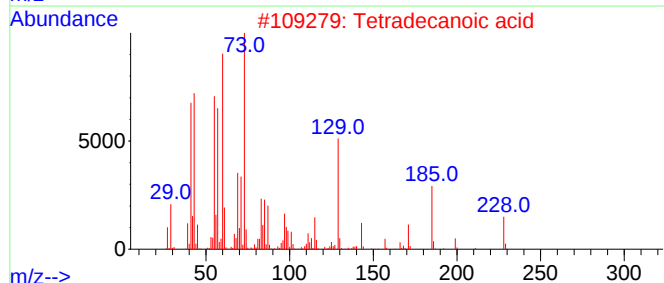
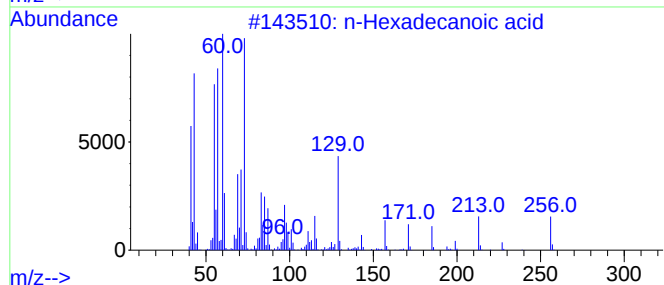
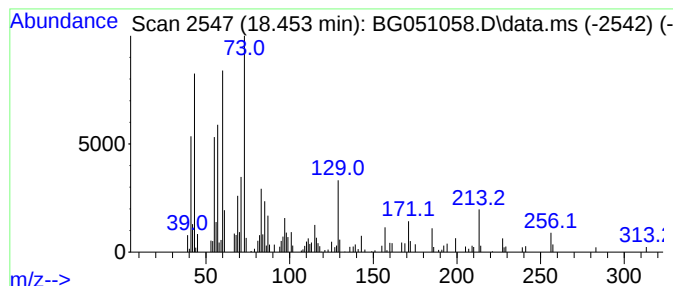
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.453	3.86 ng	127256	Phenanthrene-d10	17.601

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	97
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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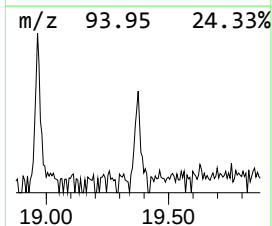
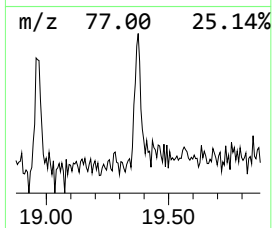
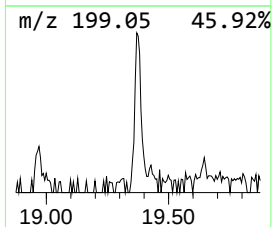
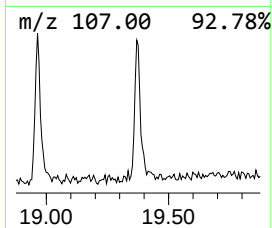
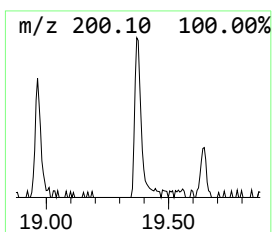
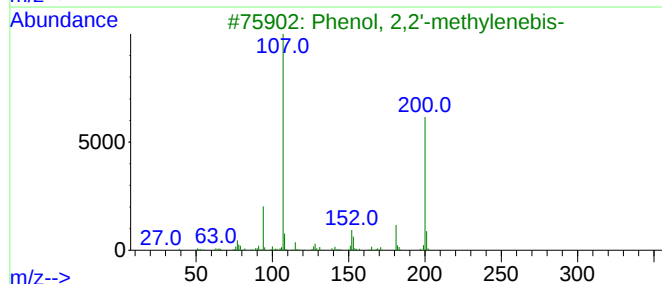
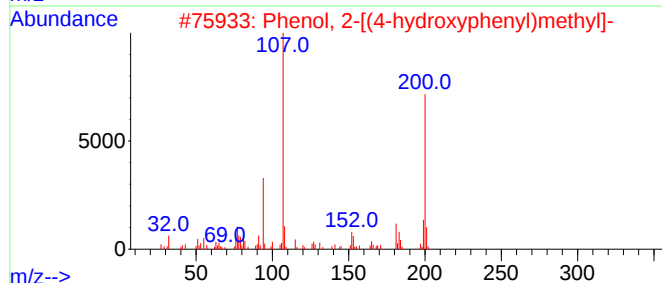
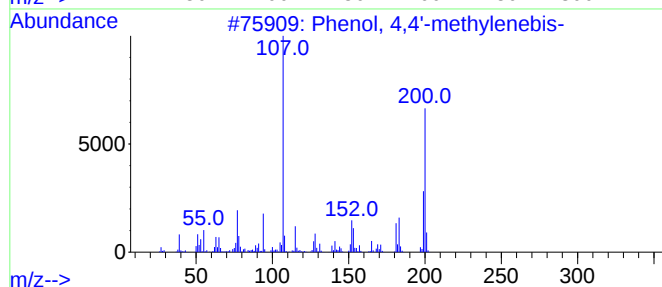
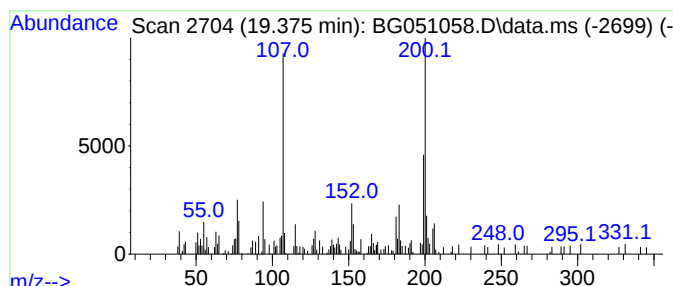
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Peak Number 4 Phenol, 4,4'-methylenebis- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.375	2.39 ng	78921	Phenanthrene-d10	17.601

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	93
2			Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	58
3			Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	58
4			1,3-Benzenediol, 4-(phenylmethyl)-	200	C13H12O2	002284-30-2	50
5			Thiazolo[5,4-f]quinoline, 7-methyl-	200	C11H8N2S	003119-56-0	38



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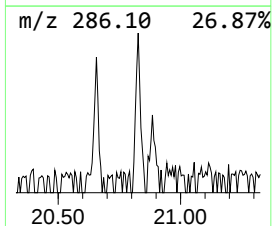
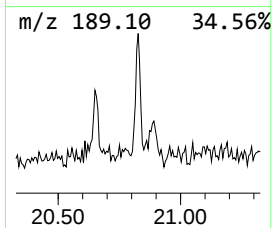
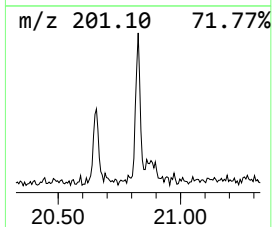
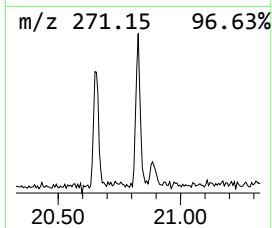
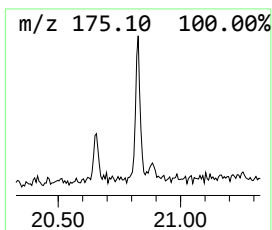
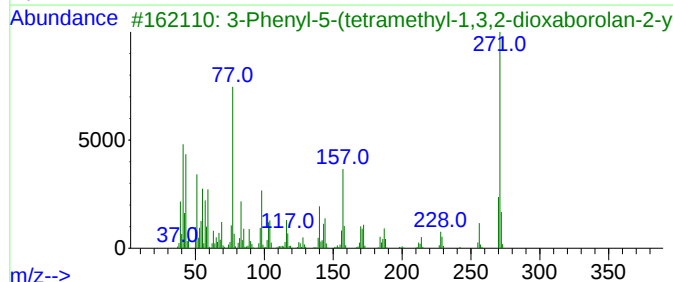
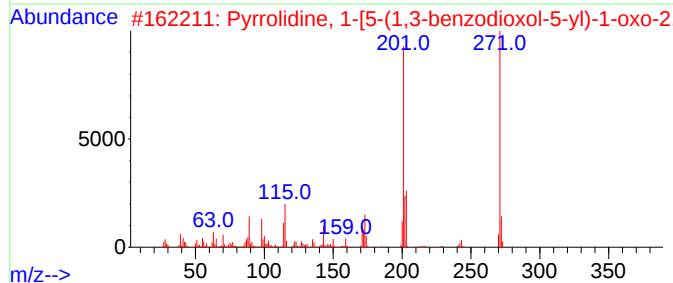
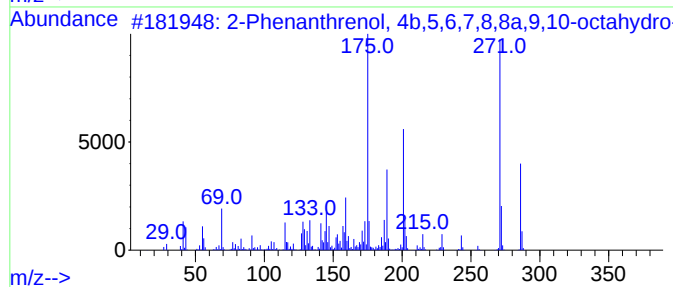
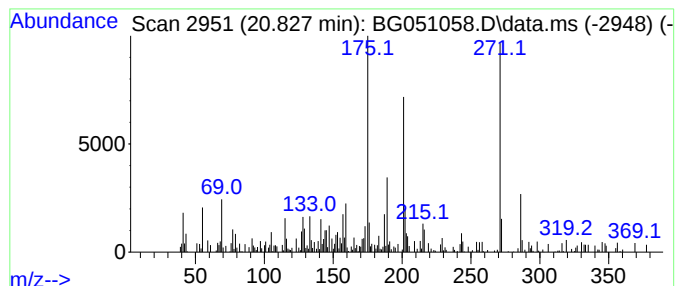
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Peak Number 5 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.827	2.03 ng	56106	Chrysene-d12	21.902

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	91		
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	45		
3	3-Phenyl-5-(tetramethyl-1,3,2-di...	271	C15H18BN03	1000434-90-0	35		
4	Naphthalene, 1,2,3,4-tetrahydro...	244	C18H28	029577-17-1	25		
5	2,2-Bis(4'-methoxyphenyl)-2-etho...	286	C18H22O3	1000283-53-7	25		



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VWE-B31-111121-10-15

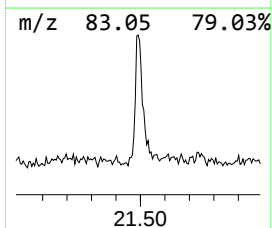
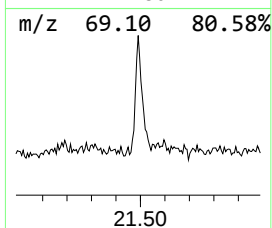
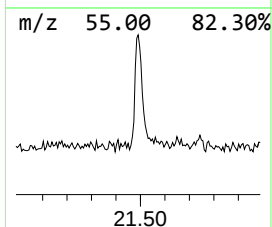
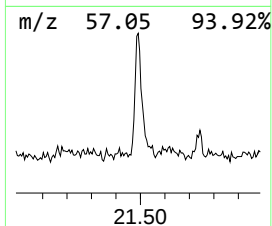
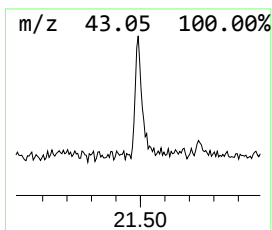
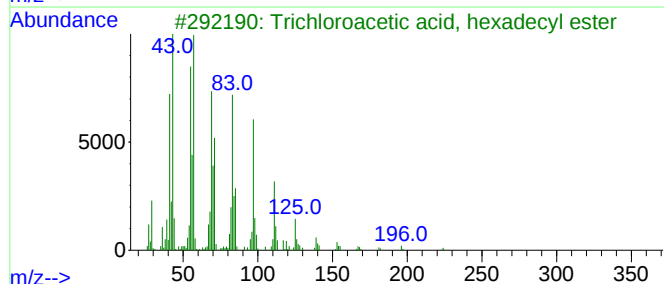
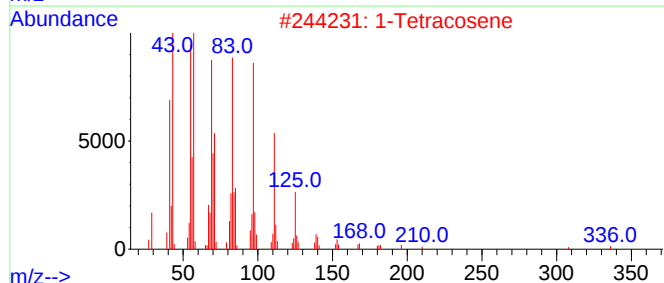
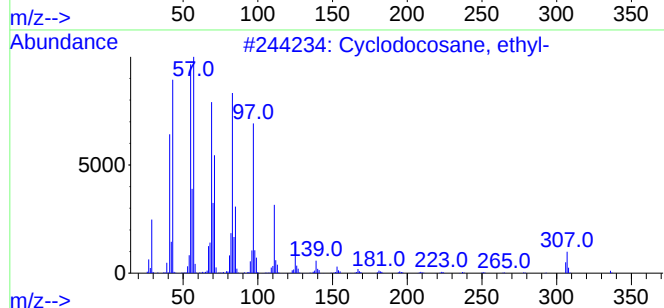
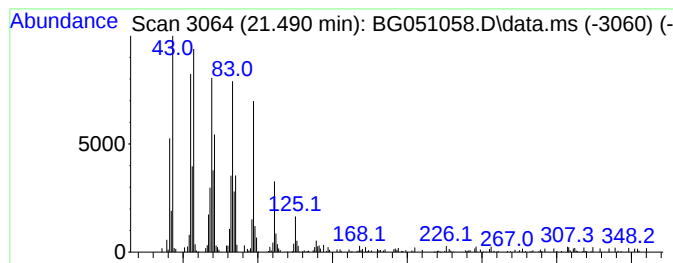
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclodocosane, ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.491	7.00 ng	193849	Chrysene-d12	21.902

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	94
2			1-Tetracosene	336	C24H48	010192-32-2	91
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5			1-Heptacosanol	396	C27H56O	002004-39-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051058.D
Acq On : 16 Nov 2021 2:13
Operator : CG/JU
Sample : M4657-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

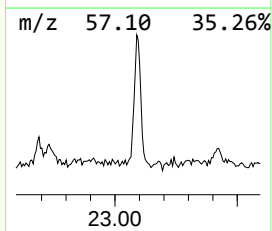
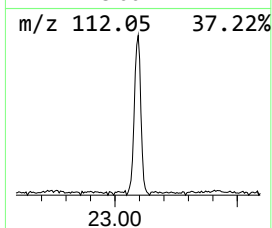
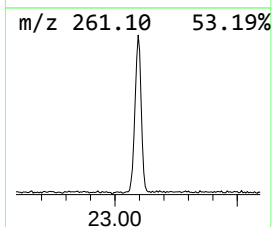
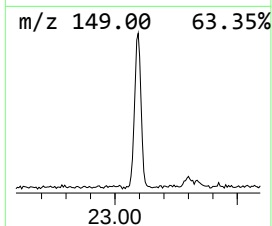
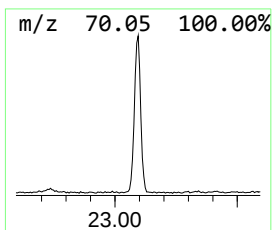
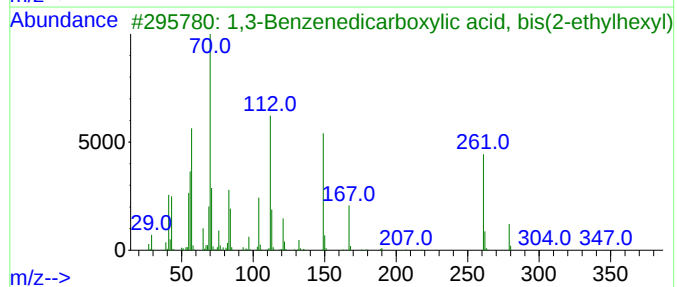
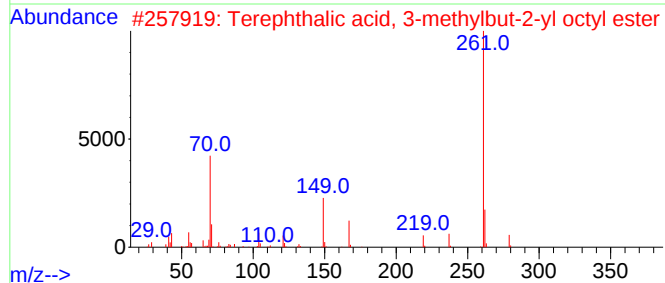
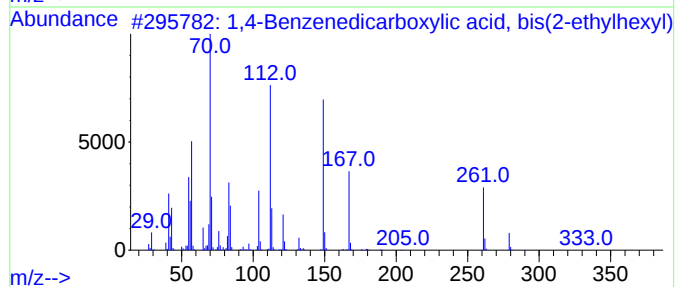
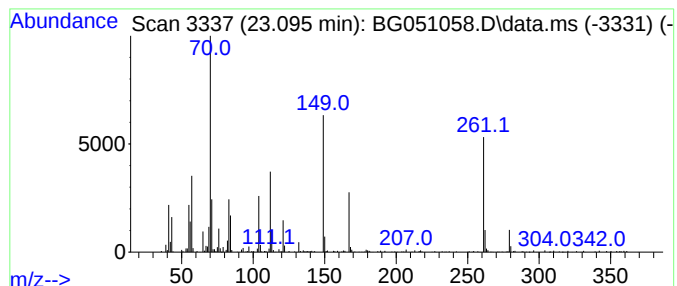
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ClientSampleId :
VWE-B31-111121-10-15

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
23.095	14.83 ng	410643	Chrysene-d12	21.902		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	59
2		Terephthalic acid, 3-methylbut-2...	348	C21H3204	1000356-27-6	50
3		1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	46
4		Isophthalic acid, di(4-octyl) ester	390	C24H3804	1000344-04-3	43
5		Terephthalic acid, 3,5-difluorop...	390	C22H24F204	1000324-05-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051058.D
Acq On : 16 Nov 2021 2:13
Operator : CG/JU
Sample : M4657-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VWE-B31-111121-10-15

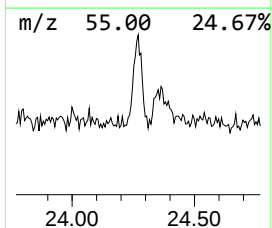
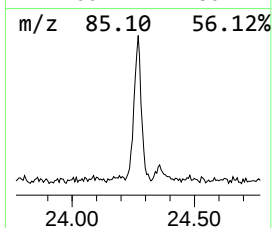
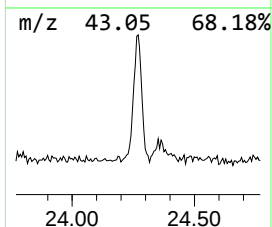
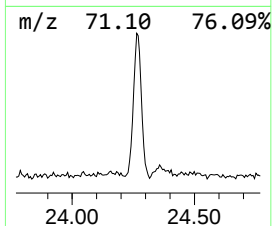
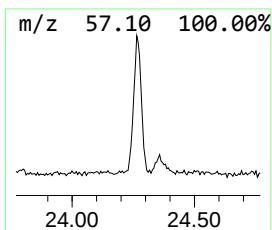
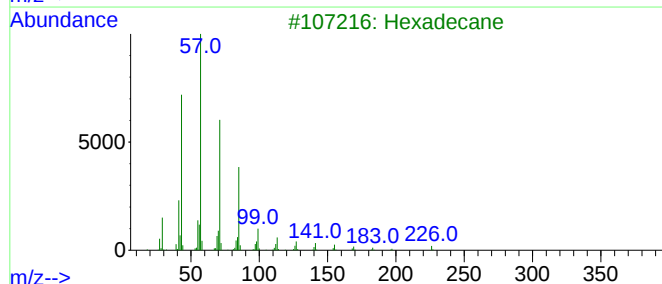
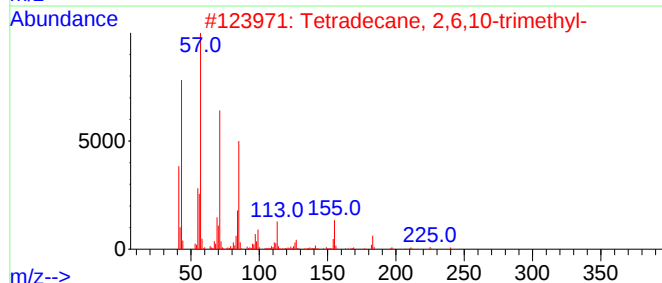
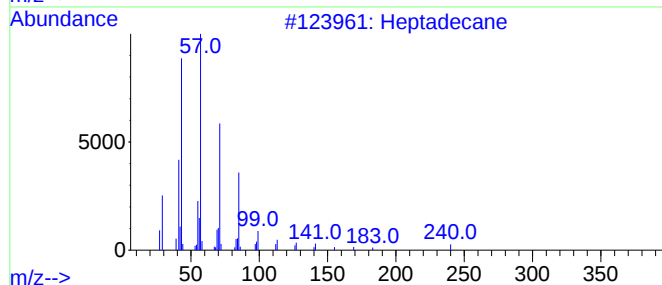
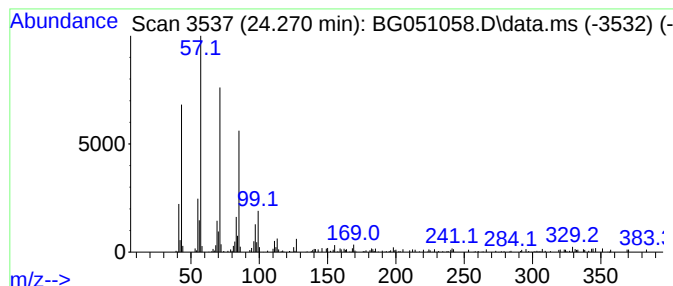
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.270	9.47 ng	213659	Perylene-d12	25.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	90
2		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	80
3		Hexadecane	226	C16H34	000544-76-3	72
4		Decane, 5-propyl-	184	C13H28	017312-62-8	58
5		Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051058.D
Acq On : 16 Nov 2021 2:13
Operator : CG/JU
Sample : M4657-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VWE-B31-111121-10-15

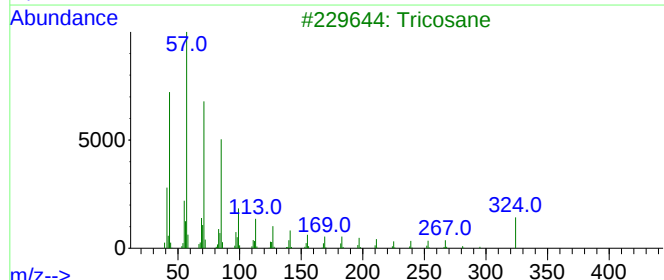
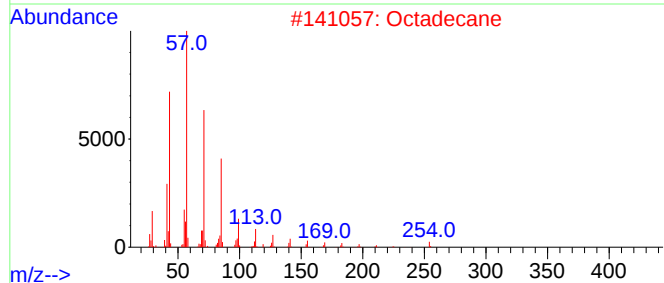
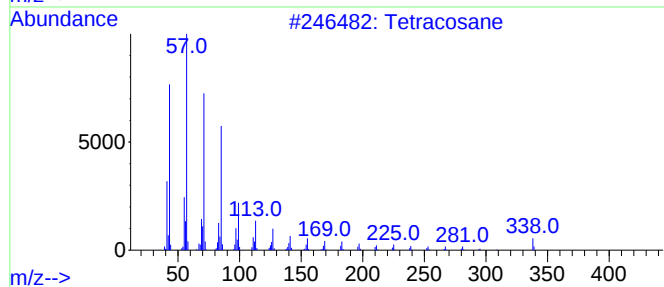
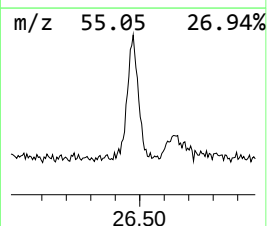
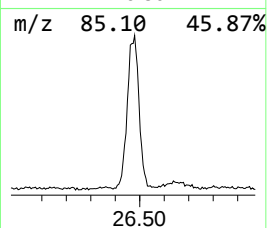
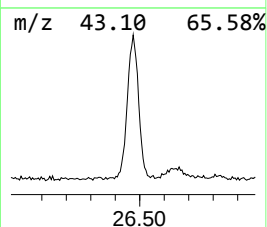
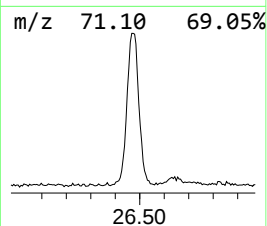
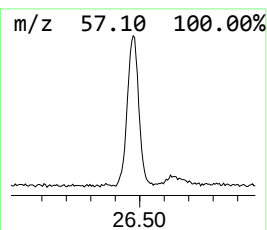
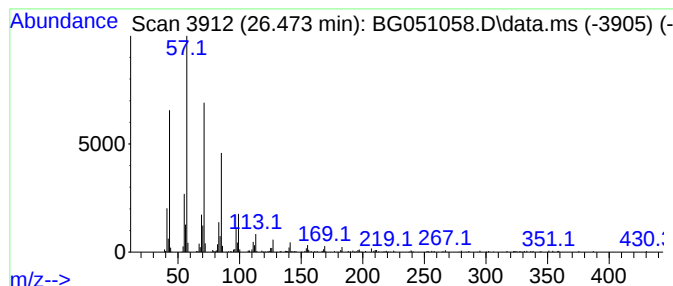
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Tetracosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.473	31.26 ng	705253	Perylene-d12	25.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	95
2			Octadecane	254	C18H38	000593-45-3	95
3			Tricosane	324	C23H48	000638-67-5	93
4			Hexacosane	366	C26H54	000630-01-3	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051058.D
Acq On : 16 Nov 2021 2:13
Operator : CG/JU
Sample : M4657-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VWE-B31-111121-10-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Ethanol, 2-(2-b...	10.797	5.5	ng	121247	2	11.056	443886	20.0
n-Hexadecanoic ...	18.453	3.9	ng	127256	4	17.601	659473	20.0
Phenol, 4,4'-me...	19.375	2.4	ng	78921	4	17.601	659473	20.0
2-Phenanthrenol...	20.827	2.0	ng	56106	5	21.902	553690	20.0
Cyclodocosane, ...	21.491	7.0	ng	193849	5	21.902	553690	20.0
1,4-Benzenedica...	23.095	14.8	ng	410643	5	21.902	553690	20.0
Heptadecane	24.270	9.5	ng	213659	6	25.310	451203	20.0
Tetracosane	26.473	31.3	ng	705253	6	25.310	451203	20.0